VSEPR and Predicting Molecular Geometry

Once we have the Lewis structure, we have the information needed to predict the geometry. It's important to remember that what we really want to know is the molecular geometry—the positions of the nuclei in relation to each other. The molecular geometry is dependent on the electron domain geometry; that is why the initial step is drawing the appropriate Lewis structure! As noted above, the simple concept behind valence shell electron pair repulsion theory (VSEPR) is the idea that electron pairs in the valence shell of an atom will repel each other and arrange themselves as far apart as possible. This arrangement of electron pairs will determine the geometry of the molecule or polyatomic ion.

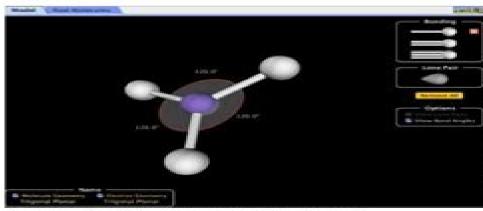


Figure 1. The PhET Computer Simulation "Molecule Shapes".

Table 2. Model Electron Domain Geometries.

Number of Electron Domains	Electron Domain Geometry	Bond Angles
2	Linear	180°
3		
4		
5		
6		

Your initial task in this activity is to determine the molecule geometry as the number of electron pairs changes. Accomplish this by using the computer simulation "Molecule Shapes" (shown at left) and fill in the table.

Notice, in this simulation you can increase the number of electron domains by adding single, double, or triple bonds, or lone pair electrons. In the lower left corner you will find both the molecule geometry and the electron geometry.

Phet Molecular Shape Simulation Answers

Ronald J Gillespie, Istvan Hargittai

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